

Overview of Accelerator Physics R&D at Tech-X

Ilya Pogorelov Tech-X Corp. (Boulder, Colorado)



SIMULATIONS EMPOWERING YOUR INNOVATIONS



Outline

- Tech-X background
- •Our software: Vorpal and VSim, USim
- •Research areas:
 - improved algorithms
 - electron cooling
 - photonics
 - LPA
- Possibilities for collaboration



Tech-X Corporation Facts

- ~30 people, 2/3 PHDs, Boulder, Colorado
- Founded in 1994
- Multiple computational physics products
- Providing services for big data distribution, management, and visualization
- http://www.txcorp.com

TECH-X Relevant Areas of Expertise

- Domains: accelerator physics, plasma physics, vacuum electronics, solid state devices
- High-performance computational software for Simulation and Design for Science and Engineering
- Enhancing code performance through porting to modern hardware (GPUs, MIC)
- High-performance visualization and graphical user interfaces
- Parallel data analysis of simulation and sensor data

TECH-X Partners and Collaborators

Our partners and collaborators are at the leading edge of science and technology. They represent a broad spectrum of efforts to discover, describe, predict and exploit the complex behaviors of matter and energy.





Customers

We provide our customers with both off-the-shelf and customized solutions addressing their advanced technology needs.



Tech-X has or had many projects with the national laboratories

- SRF cavity modeling (JLab, H. Wang)
- Modeling in support of coherent electron cooling system design (BNL, V. Litvinenko)
- Improved speed of spin tracking (BNL, M. Bai)
- Ion beam charge stripping (FRIB/MSU, F. Marti)
- GPU-accelerated ELEGANT (ANL, M. Borland)
- Prediction of beam generation in laser-plasma interactions (LBNL, W. Leemans)
- Electron cloud predictions (FNAL, Lebrun)
- Research capabilities rely heavily on our software base



Tech-X Software



VSim Family of Products: Electromagnetic and Kinetic Plasma Modeling

- VSim for Electromagnetic solutions
 - Antennas
 - Accelerator cavities
 - Photonic devices

VSim for Microwave Devices

- S-parameters
- Multipacting impacts on performance
- VSim for Plasma Discharges
 - Plasma processing
 - Plasma medical devices
- VSim for Plasma Accelerator
 - Laser-plasma wakefield acceleration
 - Beam-plasma acceleration

Vorpal is the Vsim engine: a multiphysics simulation software for modeling the interaction of matter with electromagnetic fields.







New, embedded boundary dielectric algorithm gives 2nd order error

- Traditional thinking: one must go to a finite-element method to get reasonable accuracies
- Recent results: embedded boundaries (regular meshes but special cells where cut by boundary) are both accurate and fast
 - 100x fewer operations
 - regular memory access

G.R. Werner, C.A. Bauer, J.R. Cary, A More Accurate, Stable, FDTD Algorithm for Electromagnetics in Anisotropic Dielectrics,

J. Comput. Phys. 255, (2013) 436.







C. A. Bauer, G. R Werner, and J. R. Cary, *A second-order 3D electromagnetics algorithm for curved interfaces between anisotropic dielectrics on a Yee mesh*, J. Comput. Phys. **230**, 2060-2075 (2011),



USim: Fluid and Plasmas Modeling Based on Multifluid Approach and Unstructured Meshes

USim Hypersonics

- Navier-Stokes with anisotropy
- Reaction chemistry
- Multiple species
- Real gas equation of state
- Interface to general equation of state packages
- USim High Energy Dense Plasmas
 - Gas dynamic MHD
 - Separate evolution of electrons and ions
 - General equation of state
 - Full Maxwell's equations







USim: Advanced Fluid, Plasma and EM Modeling on Unstructured Meshes

•General purpose, highresolution shock capturing methods for fluid plasma modeling on unstructured meshes

•Supports hydrodynamics, magnetohydrodynamics, Hall magnetohydrodynamics, twofluid plasmas, Navier-Stokes and Maxwell's equations •Multi-species, multitemperature versions of fluid models



DB: 8ietB-half 22.ht



Sample research projects



Modeling of coherent and conventional electron cooling



- - CeC theory is well developed:
 Ya. Derbenev, "Use of an Electron Beam for Stochastic Cooling," COOL'07 2007)
 - V.N. Litvinenko and Ya. S. Derbenev, "Free Electron Lasers and High-Energy Electron Cooling," Report BNL-79509-2007-CP (2007). V.N. Litvinenko and Ya. S. Derbenev, "Coherent Electron Cooling," Phys.
 - Rev. Lett. 102 (2009), 114801.
- Many complicating effects are best studied numerically:

 Collective effects (e.g., space charge)
 Non-uniform and non-constant electron beam density
 Finite-extent of the electron beam

 - External focusing fields
 Fully 3D simulation



δf -PIC approach results in 'cleaner' and faster simulations of the CeC modulator



δf PIC algorithm required to see signal over numerical noise



• Dynamic response extends over many λ_D and $1/\omega_{pe}$

S.E. Parker and W.W. Lee, Phys Fluids B5, 77(1993),
Q. Qian et al., Phys. Plasmas 4, 1915 (1997),
N. Xlang et al., Phys. Plasmas 13, 062111 (2006),
B.T. Schwartz et al., Proc. SciDAC Conf. (2010)
G.I. Bell et al., Proc. IPAC, THEPPB002 (2012)

S2E coupled Vorpal-Genesis simulations yield the most accurate **BROOKHAVEN** computation of the kick on the ion

- 3D simulations of anisotropic Debye shielding coupled to 3D FEL simulation with Genesis and ES PIC simulation of the kicker with Vorpal
- Start-to-end simulation enables parametrization of the kick on the ion

B.T. Schwartz et al., Proc. PAC, MOP074 (2011) B.T. Schwartz et al., Proc. IPAC, MOPWO071 (2013)

Below: Kick on a gold ion, initially stationary in beam frame, then moving backwards longitudinally





Variation of $E_z(z)$ in kicker over one plasma period



Kick on the ion depends on its longitudinal velocity,

BCC algorithm allows rigorous CECH-X COMPUTATION OF DYNAMICAL Friction

- Model a single pass (as opposed to cooling on macroscopic timescales); simulations are done in the beam frame
- Focus on detailed dynamical friction computation with Vorpal that resolve individual ion-electron collisions
- Binary Coulomb collision (BCC) model is a variant of N-body solver based on exact solution to 2-body collisions with artificial suppression of diffusion [G.I.Bell et al., J. Comp. Phys. 227, 8714-8735 (2008)]
- Arbitrary external fields can be taken into account via an operator splitting technique that preserves 2nd-order accuracy
- Correctly accounts for finite-interaction-time effects, details of the electron distribution; no assumptions of working in a particular asymptotic regime
- Enabled a greatly improved understanding of small impact parameter collisions, including a generalization of the Coulomb logarithm, and was used for cross-checking with existing (semi-)analytic models

δf-PIC in Vorpal simultaneously captures **CECH-X dynamical friction and electron response**

- Vlasov-Poisson description, ion shielding by electrons treated as a perturbation, artificial diffusion suppression not needed
- In the frame where ion is initially at rest, we compute the electric field due to the wake at the ion location to get friction force
- A grid is required for the Poisson solve, effectively limiting the timestep
- A notable advantage: particle noise in a δf -based computation is greatly reduced compared with the binary collision model
- Simultaneously captures the ion dynamics (dynamical friction) and bulk electron response (Debye shielding)





Dielectric accelerating structures





- Dielectric Laser Accelerators have the goal of making use of the high laser power
- Optical (1): "The onset of breakdown, detected through light emission from the tube ends, is observed to occur when the peak electric field at the dielectric surface reaches 13.8±0.7 GV/m."
- GHz (2): experimental evidence is lacking but accelerating gradients near 10 MV/m have been observed without breakdown; multipacting currently prevents studies at higher surface fields in the DLA geometry
- M. Thompson, H. Badakov, A. Cook, J. Rosenzweig, R. Tikhoplav, G. Travish, I. Blumenfeld, M. Hogan, R. Ischebeck, N. Kirby, et al., Physical review letters 100, 214801 (2008), ISSN 1079-7114.
- 2. C.Jing,W.Gai,J.Power,R.Konecny,W.Liu,S.Gold,A.Kinkead,S.Tantawi,V.Dolgashev, and A. Kanareykin, Plasma Science, IEEE Transactions on 38, 1354 (2010)

U Dielectric systems may be <u>smaller</u>



TUYB02

Proceedings of IPAC2012, New Orleans, Louisiana, USA

- If one gets breakdown at 10 GeV/m, then 100x shorter
- As seen at right, much narrower
- Smaller (µm sized) structures have been fabricated
 - Wood pile
 - Dielectric fibers

MANUFACTURE AND TESTING OF OPTICAL-SCALE ACCELERATOR STRUCTURES FROM SILICON AND SILICA*

R. J. England, E. R. Colby, R. Laouar, C. M. McGuinness, B. Montazeri, R. J. Noble,
E. A. Peralta, K. Soong, J. Spencer, D. Walz, Z. Wu, SLAC, Menlo Park, CA 94025, USA
M. Qi, C. Lee, Y. Xuan, L. Fan, L. T. Varghese, Purdue Univ., West Lafayette, IN 47907, USA
R. L. Byer, C-M. Chang, K. J. Leedle, Stanford Univ., Stanford CA, USA
B. Cowan, Tech-X, Boulder CO, USA



Figure 1: Three dielectric laser accelerator topologies: (a) a 3D silicon photonic crystal structure, (b) a hollow-core photonic bandgap fiber, and (c) a dual-grating structure, showing conceptual illustration (top) and recently fabricated structures (bottom).



- Demonstrated high-efficiency coupling to a photonic crystal accelerating waveguide — over 90% power efficiency into the forward direction
- Efficiency improved by adjustments of individual rods
- Geometry adjustments amenable to lithographic fabrication
- Structure designed by parameter scans with high-performance Vorpal simulations



Laser-Plasma Acceleration

Controlled dispersion gives more accurate Injection stage simulations

- More physical, better converged results in quasilinear stage simulations
- More physical injection model: Injected beam dephases more slowly, gains more energy



B. Cowan *et al.*, PRST-AB **16**, 041303 (2013) B. Cowan *et al.*, J. Plasma Phys. **78**, 469 (2012) SIMULATIONS EMPOWERING YOUR I



Enhanced loading improves accuracy of injected electron bunches

- Load greater particle statistics in collection volume where injected electrons originate
- Convergence demonstrated in injected bunch parameters
- Reveals, clarifies features in transverse phase space



ECH-X Beam-frame Poisson solve algorithm eliminates numerical emittance growth

- Self-fields of the e⁻ bunch can be found from a Poisson solve in the beam frame; very similar to what is done in tracking codes
- The beam self-fields are calculated at each time step using a Poisson solver in the frame of the moving beam
- EM PIC shows artificial emittance growth even with aggressive smoothing and higher resolution; BFPS eliminates





Working with Tech-X

Work with Tech-X to tap substantial SBIR/ STTR program

- Mandated by Congress
- \$21 billion in research, 400k scientists and engineers 1982-2009
- Fraction of research funding (not construction, NNSA exception)
 - ◆ SBIR: 2.6% in 2012 to 3.2% in 2017
 - STTR: .35% for 2012 and 2013 to
 - 0.45% in 2016
- Staged approach
 - Phase I: \$150k for 9 months
 - Phase II: \$1M for 2 years
- OR Fast track: All in one go

Increasing emphasis on commercialization implies agency, dual, or pure comm use

- Prior to reauthorization: producing something that the agency (e.g., for its lab infrastructure) wanted was enough
- Since reauthorization, one must show strong potential for commercialization, e.g.,
 - Agency purchase
 - Agency follow-on funding
 - Private sector funding or purchase
- Venture backed firms may now participate in the SBIR program
- DOE needs to learn how to take advantage of SBIR while ensuring commercialization or any benefit of funds to research mission may be lost



- Lab identifies something it needs and will acquire
- Marketplace not currently meeting the need
- Need exists beyond the lab
- Examples:
 - Design tools for accelerators
 - Computational appliance: custom computer with HPC software installed, e.g., GPU capable
 - Data acquisition boards
- Lab uses SBIR to get the initial R&D done and shapes the product through its involvement
- Lab acquires the product that it wanted



Thanks! LOOKING FORWARD TO COLLABORATION!



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Removed

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Vorpal has the speed of FDTD with the accuracy of finite-element methods

Maxwell discretized by finite difference

$$\frac{\partial \mathbf{E}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\frac{\partial \mathbf{E}}{\partial t} = c^{2} \left[\nabla \times \mathbf{B} - \mu_{0} \mathbf{j} \right]$$

$$B_{x,i,j,k}^{n+1/2} - B_{x,i,j,k}^{n-1/2} = \Delta t \left(\frac{E_{z,i,j,k}^{n} - E_{z,i,j+1,k}^{n}}{\Delta y} + \frac{E_{y,i,j,k+1}^{n} - E_{y,i,j,k}^{n}}{\Delta z} \right)$$

$$E_{z,i,j,k}^{n+1/2} = \Delta t \left(\frac{E_{z,i,j,k}^{n} - E_{z,i,j+1,k}^{n}}{\Delta y} + \frac{E_{y,i,j,k+1}^{n} - E_{y,i,j,k}^{n}}{\Delta z} \right)$$

Same for E; Yee mesh \

aR

- Regularly structured data is desired:
 - Best for access, especially on modern architectures
 - Works well with particles if rectilinear
- Conformal (curved) surfaces are represented by embedded boundaries

 R^{ijk}

TECH-X Fast through use of structured meshes

- Traditional unstructured-mesh approach, accurate with curved boundaries, minimizes operations but not well adapted to todays' processors (CPU, Phi, GPU)
- Computations on structured meshes are fast on today's processors
 - Regular memory access
 - Ideal for vector processing



We can now get the access speed of structured meshes with the accuracy of unstructured!



Distributed memory and implicit algorithms shorten time to solution

- Application spans multiple processors, each solving a region of the problem
- MPI used to pass boundary information between the processors
- Good scaling shows ability to solve problem requiring very large memory in reasonable time





- One can get absolute numerical stability by having the solution at the advanced time depend on itself.
- This requires that one solve an implicit equation (the solution is defined implicitly as a function of itself)
- Result: ability to step over orders of magnitude of uninteresting dynamics

SIMULATIONS EMPOWERING YOUR INNOVATIONS

TECH-X In-memory multiphysics through TruCouple™

- Implemented within VSim
- "Assembly language for Partial Differential Equations"
- Allows one to compose fast coupling of any number of fields, with particles, even defining the equations and coupling in the input file while having the speed of compiled code
- Unique capability in distributed memory computing
- Applications
 - Coupled electromagnetic/plasma
 - Coupled multi-component plasma
- Developing EM-thermal coupling

USim: Advanced Fluid, Plasma and EM Modeling on Unstructured Meshes

The USim advantage:

•All physics models can be solved on structured, body fitted and unstructured meshes in multidimensions

•Cartesian, Spherical and Cylindrical coordinate systems

•Examples and documentation for each physics and algorithm option gets results faster.

•USimComposer allows simulation validation, execution and visualization in one application.

•Works for:

•single and multi-core systems.

•Windows, MacOS and Linux operating systems.



Hypersonic flow with accelerated Navier-Stokes and chemistry



Multi-dimensional shocks over simple geometries

SIMULATIONS EMPOWERING YOUR INNOVATIONS

Work with us on existing product line or to develop a new one

- VSim for Electromagnetic solutions
 - Antennas
 - Accelerator cavities
 - Photonic devices
- VSim for Microwave Devices
 - S-parameters
 - Multipacting impacts on performance
- VSim for Plasma Discharges
 - Plasma processing
 - Plasma medical devices
- VSim for Plasma Accelerator
 - Laser-plasma wakefield acceleration
 - Beam-plasma acceleration



- USim Hypersonics
 - Navier-Stokes with anisotropy
 - Reaction chemistry
 - Multiple species
 - Real gas equation of state
 - General equation of state
- USim High Energy Dense Plasmas
 - Gas dynamic MHD
 - Separate evolution of electrons and ions
 - General equation of state
 - Full Maxwell's equations
- GPULib: High-performance IDL addon
- PTSolve: high-performance math libraries
- PyDDS: Python bindings for the data distribution service



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Basic Physics: Photonic crystals have propagation bands with gaps (band gaps)^{TECH-X}

 A 1D photonic crystal (alternating dielectric layers) is highly reflective to a normally incident wave of the right frequency, due to destructive interference.



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 2D and 3D photonic crystals (like atomic crystals but with "dielectric atoms" and lattice spacings on the order of the wavelength of interest) can be tailored to reflect waves within a certain frequency bandgap, regardless of their angle of incidence or polarization.

th d lattice of the t) can be es within a dgap, gle of ion.



A beam of charged particles excites high order modes in an accelerating cavity that, unless sufficiently damped, diminish the quality of following particle bunches.

If the cavity walls have a PhC at the cavity's resonant frequency, the cavity will have a high Q at that frequency, but frequencies not in the PBG will pass harmlessly out of the cavity.





Two directions of current photonic cavity research

RF

- Claddings
- 2D rod arrays
 - Metallic
 - Dielectric

Optical

- Dielectric fibers
- 3D structures like woodpiles
- Gratings

Have common goals

- Reduce wake fields (Stable)
- Improve coupling
- Increase breakdown voltage





- Q larger by 2 orders of magnitude for optimized 18 rods compared with best truncated 18-rod crystal
- Q larger for optimized 18 rods by one order of magnitude compared with 147 rods in truncated crystal
- For 24 rods, we find vacuum Q of 10⁵: 100x improvement in Q, 1/6 the number of rods, ¹/₄ the volume!

STUDY OF HYBRID PHOTONIC BAND GAP RESONATORS FOR PARTICLE ACCELERATORS

M. R. Masullo,¹ A. Andreone,² E. Di Gennaro,² S. Albanese,³ F. Francomacaro,³ M. Panniello,³ V. G. Vaccaro,³ and G. Lamura⁴

2486 MICROWAVE AND OPTICAL TECHNOLOGY LETTERS / Vol. 48, No. 12, December 20

room temperature confirm the monomodal behavior, but the Q value is lower than expected (roughly 10^3). This is mainly due to





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A single pass through the CeC **BROOKHAVEN** cooling system

Hadrons **Electrons** High gain FEL (affects electrons only) 22 MeV Electron **Modulator** FEL **Kicker** Linac Amplifier High-gain FEL operate in Self-• The ions respond to fields of Anisotropic Debye shielding **Amplified Stimulated-Emission** the amplified electron density occurs for each ion. perturbation, resulting in an

- The coherent density/velocity modulation is typically smaller than shot noise
- Non-linear effects are small, so that noise and ion signal are assumed to be additive.

Amplified Stimulated-Emission (SASE) mode.
The wiggler is short enough to avoid saturation so that the output of the

- saturation so that the output of the FEL (amplified density and energy modulations) obeys linear Vlasov theory.
- The amplified noise and "cross-talk" results in incoherent signal
- The amplified bunching from screening results in a coherent signal for each ion (as for stochastic cooling).
- Linear perturbations of the beam-frame "plasma" evolve for about 0.25 plasma periods.

effective velocity drag.





CeC cooler components require different simulation tools





- Must be able to accurately model 3D anisotropic Debye shielding with low numerical noise in external fields
- Should ideally be able to use multiple algorithms
- BEST SOLUTION:
 - δf Particle-In-Cell (PIC) in the Beam-Frame

Vorpal

- Must be able to model SASE singlepass FEL designs (large multi-scale problem)
- Must be time-dependent and 3D
- Must be able to take output from Modulator as input, and provide output for kicker simulations
- BEST SOLUTION:

Specialized SASE single-pass FEL code in the Lab Frame





- Similar requirements as for Modulator, but not as demanding...
- BEST SOLUTION:

Electrostatic Particle-In-Cell (PIC) in the Beam-Frame





3D δf -PIC modulator simulations successfully validated



Simulated e- density agrees with theory



Drifting ion simulations agree w/ theory [7]



Maxwellian wakes can differ from Lorentzian



Large transverse drift velocity yields strongly perturbed wakes over many Debye lengths



ion

- Analytic theory makes certain assumptions:
 - Single ion, with arbitrary velocity
 - Uniform e⁻ density; anisotropic temperature
 - Lorentzian velocity distribution
 - Linear plasma response
- Theory is computed from:

G. Wang and M. Blaskiewicz, Phys. Rev E 78, 026413 (2008).

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Single-pass frictional cooling simulations

- Model a single pass (as opposed to cooling on macroscopic timescales); simulations are done in the beam frame
- Focus on detailed dynamical friction computation with Vsim (Vorpal) that resolve individual ion-electron collisions
- Take into account finite interaction time effects, details of the electron distribution; no assumptions of working in a particular asymptotic regime
- Useful for cross-checking with existing (semi-)analytic models
- Also for constructing new parametrized models of the dynamical friction force for numerical work
- Two simulation models implemented in Vsim: the *binary* collision and δf -PIC
- Binary collision model is a variant of N-body solver based on exact solution to 2-body collisions with artificial suppression of diffusion [G.I.Bell et al., JCP 227, 8714-8735 (2008)]



δf -PIC in VSim extended to model dynamical friction

- Vlasov-Poisson description, ion shielding by electrons treated as a perturbation [Parker and Lee, Phys. Fluids B 5, 77 (1993); Xiang, Cary and Barnes, Phys. Plasmas 13, 062111 (2006)]
- In the frame where ion is initially at rest, we compute the electric field due to the wake at the ion location to get friction force
- A grid is required for the Poisson solve, effectively limiting the timestep
- A notable advantage: particle noise in a δf -based computation is greatly reduced compared with the binary collision model



Binary Collision model

δf-PIC model